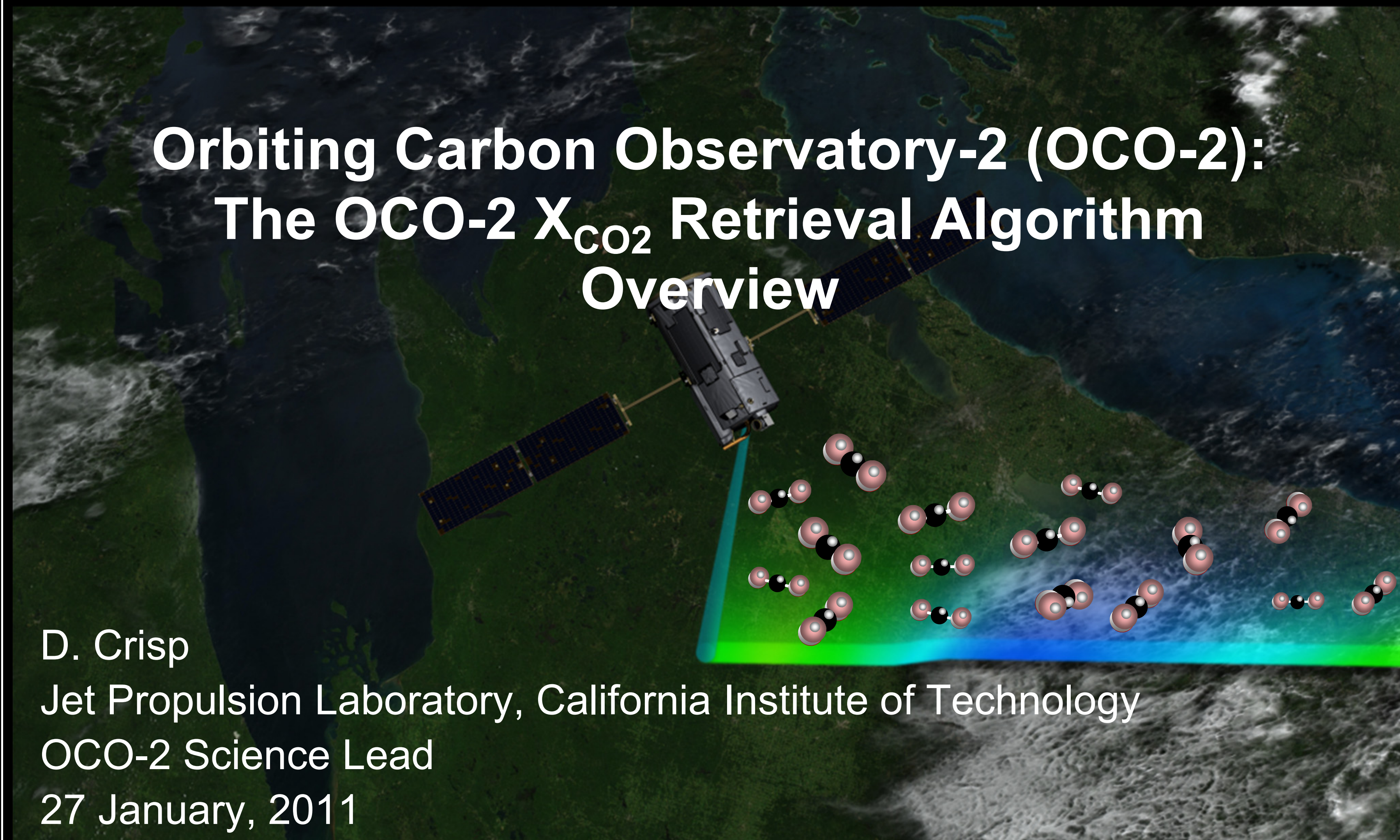
OCO-2 / MicroCarb Meeting, Caltech 27 January 2011



Orbiting Carbon Observatory-2 (OCO-2): The OCO-2 X_{CO2} Retrieval Algorithm Overview

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Retrieving X_{CO2} from Near-IR Spectra

- The primary purpose of the retrieval algorithm is to derive estimates of the column averaged atmospheric CO_2 dry air mole fraction, X_{CO2}, and other Level 2 data products from the near-IR (NIR) spectra

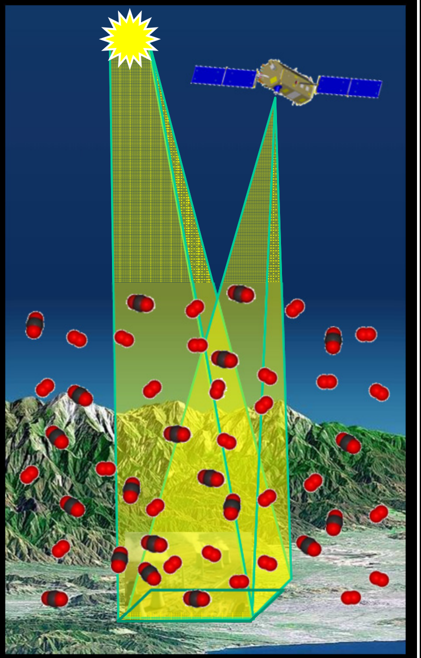
- X_{CO2} is defined as the ratio of the column abundances of CO_2 and dry air,

$$X_{CO2} = \int N_{CO2}(s)\, ds \,/ \int N_{air}(s)\, ds$$

- $N_{CO2}(s)$ is the number density of CO_2 and $N_{air}(s)$ number density of dry air at point, s, along the optical path between the sun, surface, and spacecraft

- Because O_2 constitutes 0.20955 N_{air}, X_{CO2} can also be defined as:

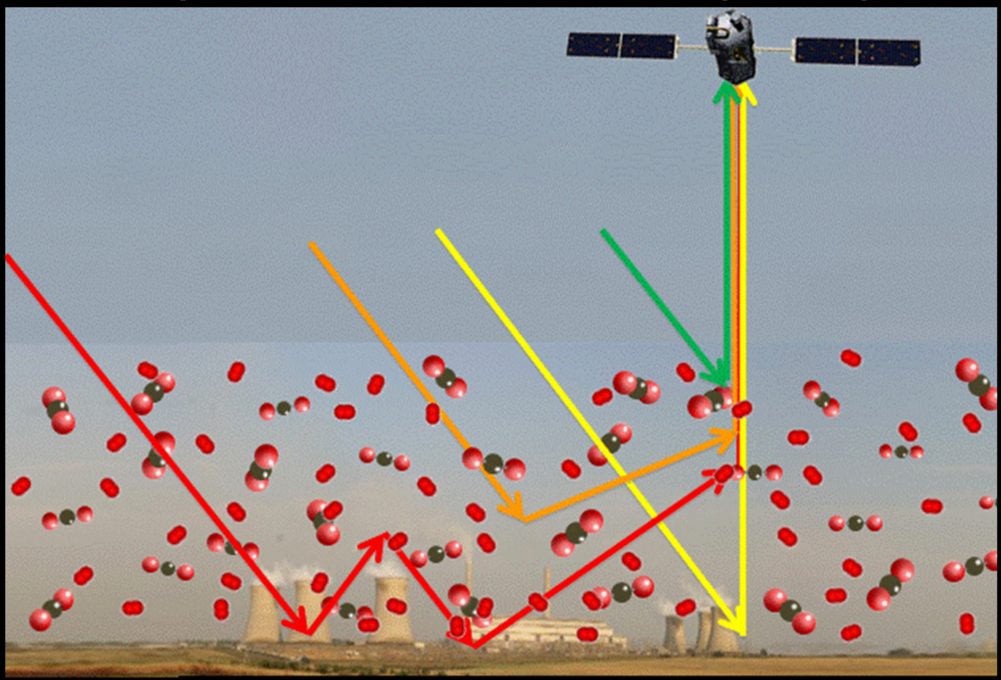
$$X_{CO2} = 0.20955 \times \int N_{CO2}(s)\, ds \,/ \int N_{O2}(s)\, ds$$

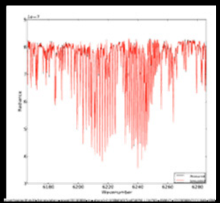


Column abundances of CO_2 and O_2 are retrieved from bore sited spectroscopic measurements of NIR CO_2 and O_2 bands

Retrieving the Number Densities from Atmospheric Absorption Measurements

- At wavelengths where CO_2 and O_2 absorb sunlight, the reflected intensity is inversely proportional to the number of molecules along the optical path
- Column densities of CO_2 and O_2 can be retrieved from NIR spectra of reflected sunlight if the wavelength-dependent absorption cross section per molecule and the optical path length are known.





Challenges:

- Gas absorption cross sections vary rapidly with wavelength
- Photons can take a wide range of paths through a scattering, absorbing atmosphere

Generic Retrieval Process

- Given an initial guess of the atmospheric structure, composition, and the surface and atmospheric optical properties and viewing geometry, a **Forward Model** is used to generate
  - a **synthetic spectrum** of the sunlight reflected by the surface and atmosphere, that fully resolves the spectral structure of the gas, aerosol, and surface optical properties
  - **Jacobians**, which describe the rate of change (first derivative) of the radiances at each spectral point with respect to each atmospheric property to be refined (e.g. number densities of CO_2, O_2, and other gases, cloud and aerosol distribution and optical properties, surface reflectance)
- The synthetic spectrum (and Jacobians) is processed with an **Instrument Model** that simulates the instruments spectral resolution and sampling, and is compared to the observed spectrum
- An **Inverse Model** uses Jacobians (and other constraints) to modify the atmospheric and surface properties to improve the fit
- The process is repeated until the convergence criteria are met

Retrieving X_{CO2} from NIR Data

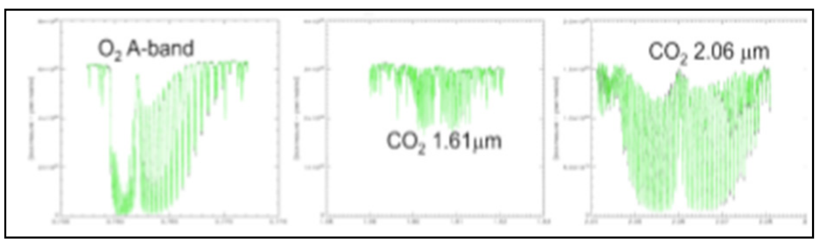
Cloud Screening Results

L1B Data

Frame ID List

Forward Model

State Vector First Guess



(Model – Obs) residuals

State Vector Apriori + Covariance

Update State Vector

- Final State Vector
- Aposteriori Covariance Matrix
- Diagnostics

The ACOS/OCO-2 Retrieval Algorithm

- Pre-processing
  - Associates meteorological and geometric data and surface/atmospheric optical property databases to define the initial surface-atmosphere state
- Pre-screening
  - Assess SNR, solar zenith angle range, surface roughness, and screen for clouds to determine if sounding is useful for XCO2 retrievals
- Forward Model
  - Combines optical property and a solar spectral databases with state information in a pseudo-spherical, spectrum-resolving multiple scattering model to generate a polarized synthetic spectrum and Jacobians
- Instrument Model
  - Convolves synthetic spectrum (and Jacobians) with instrument line shape, spectral sampling, and applies instrument polarization response
- Inverse Model
  - Uses optimal estimation to refine the atmospheric state to improve the fit between the synthetic and observed spectrum
- Post Screening:
  - Discards soundings that do not pass quality criteria

Pre-Processing: A priori Set-up Meteorology

ECMWF T799 (91 levels) 3-12hr Forecast (every 3 hrs)

- ~26 km pixels interpolated spatially & temporally to footprint.

- Temperature & specific humidity profiles, wind speed & surface pressure interpolated to fixed pressure grid.

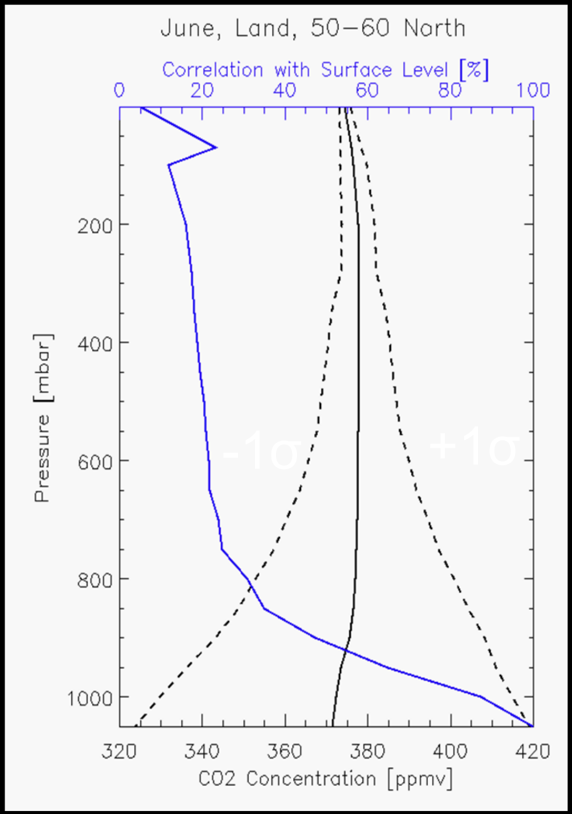
- Surface pressure additionally adjusted to footprint elevation via hydrostatic equation.

• Temperature offset:	0.0 $\pm$ 5 K
• Water Vapor Scale Factor :	1.0 $\pm$ 0.5
• Surface Pressure:	ECMWF $\pm$ 4 hPa
• Wind Speed :	ECMWF $\pm$ 10 m/s

A priori Set-up : CO_2

CO_2 profiles from LSCE Model*

- 1 yr model results binned into 10° zonal bins
- Separately for land vs. ocean
- Separately for each month
- Interpolated to FP level grid
- + Annual CO2 secular increase (NOAA ESRL)
- Covariance matrix is non-diagonal
(~ 5.7 degrees of freedom)



** Courtesy Peter Rayner*

A priori Set-up : Cloud and Aerosols

- 0.15 total cloud + aerosol optical depth.
- Cloud water: R_{eff} = 8 μm (mid trop)
- Cloud ice : R_{eff} = 70 μm (upper trop)
- 2 Kahn Aerosol types (5 & 7, lower trop)

Table 2. Climatological Mixing Groups and Representative Air Mass Types

Classification	Component 1	Component 2	Component 3	Component 4	Notes
1. Carbonaceous + dusty maritime	sulfate	sea salt	carbonaceous	accum. dust	34% of voxels are nonzero
1a	(0.67)	0.13	0.10	0.10	middle- to high-latitude oceans, winter; Nov.–May, southern oceans; May–Sept., North Atlantic
1b	0.41	0.13	(0.27)	(0.19)	tropical to subtropical oceans, all year; June–Oct., remote southern oceans
1c	0.40	(0.32)	0.17	0.11	southern midlatitude oceans, all year; Nov.–March, remote southern oceans
2. Dusty maritime + coarse dust	sulfate	sea salt	accum. dust	coarse dust	14% of voxels are nonzero
2a	(0.52)	0.17	0.21	0.10	downwind of deserts: Australia, Africa, South America, peak during southern summer; Oct.–Jan., N. W. Africa
2b	0.29	0.13	(0.39)	(0.19)	same pattern as 2a but closer to continental source regions
3. Carbonaceous + black carbon maritime	sulfate	sea salt	carbonaceous	black carbon	11% of voxels are nonzero
3a	(0.51)	0.18	0.26	0.05	ocean near Indonesia, all year; Dec.–March, North Atlantic; Jan.–Feb., oceans near central Africa; May–July, oceans near tropical South America; July–Sept., oceans near central America
3b	0.35	0.10	(0.47)	(0.08)	same pattern as 3a but closer to continental source regions

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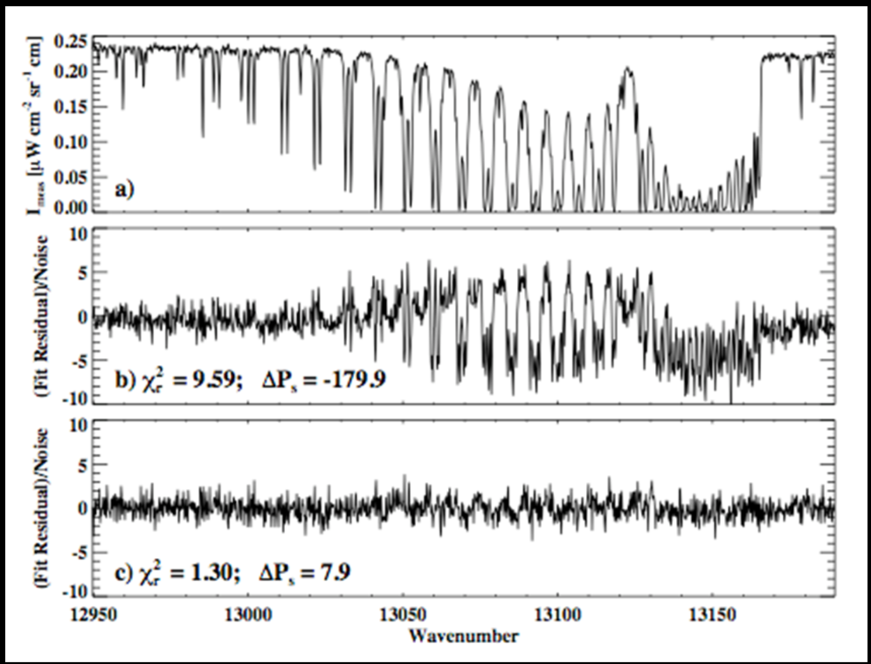
Pre-Screening: The ACOS Cloud Screen

- A Spectroscopic cloud screening algorithm based on the O_2 A-band is currently being used for GOSAT retrievals
  - Fits a clear sky atmosphere to every sounding in the O_2 A band.
  - High values of χ^2 and large differences between the retrieved surface pressure and the ECMWF prior indicate the presence of clouds
  - Over non-glint ocean, a simple albedo test is also used.



Example A-Band fit

Poor fit (χ^2 = 9.6) indicates presence of cloud

Small residuals and good agreement between retrieved and ECMWF surface pressure indicates cloud free

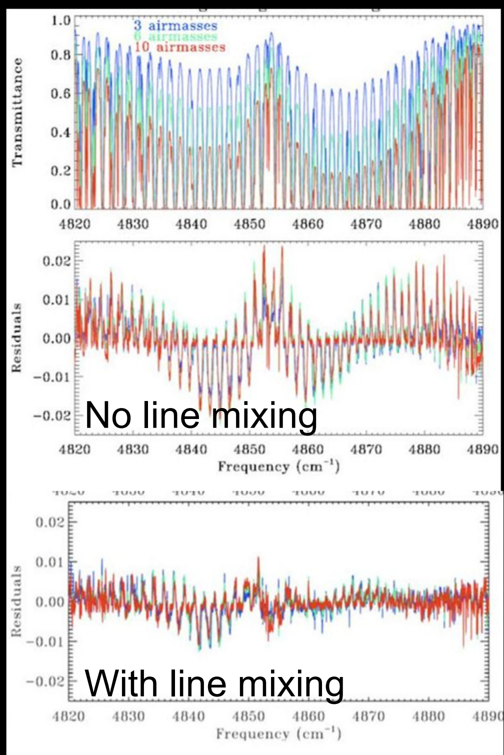
ACOS/OCO-2 Forward Model

The ACOS/OCO-2 Forward Model incorporates:

- Spectrally-dependent atmospheric optical properties module
  - Gas absorption cross-section databases
  - Rayleigh scattering cross-section
  - Cloud and aerosol single scattering optical properties databases
  - Surface reflectance
- Solar Model
  - Solar continuum
  - Solar line list
- Atmosphere/surface Radiative Transfer Model
  - Scalar multiple scattering code (LIDORT)
  - 2 Order of Scattering Polarization Correction code
- Radiance Jacobians module

Molecular Gas Absorption

- CO_2, H_2O, O_2, +isotopologues.
- Cross-section tables pre-generated and stored
- Line mixing included in all CO_2 and O_2 bands.



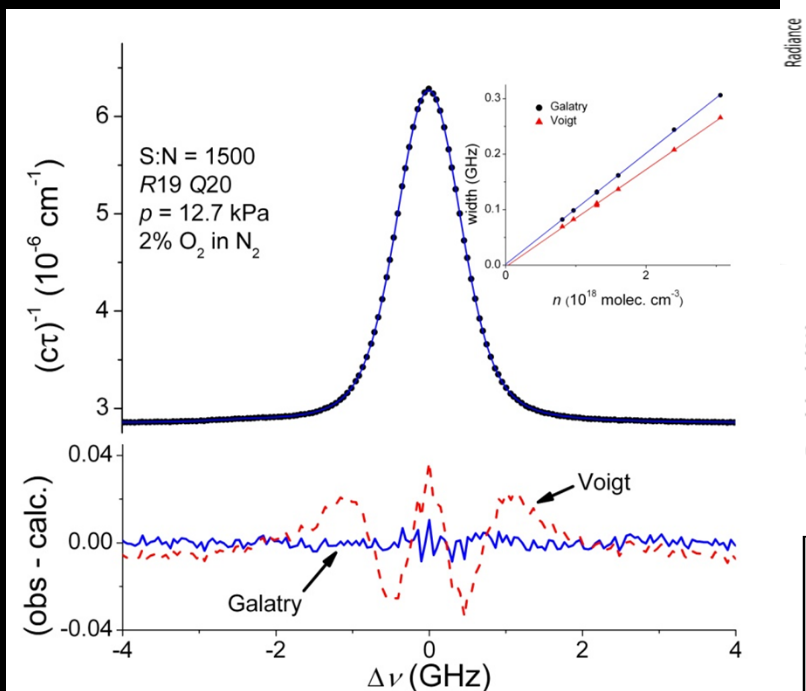
Databases

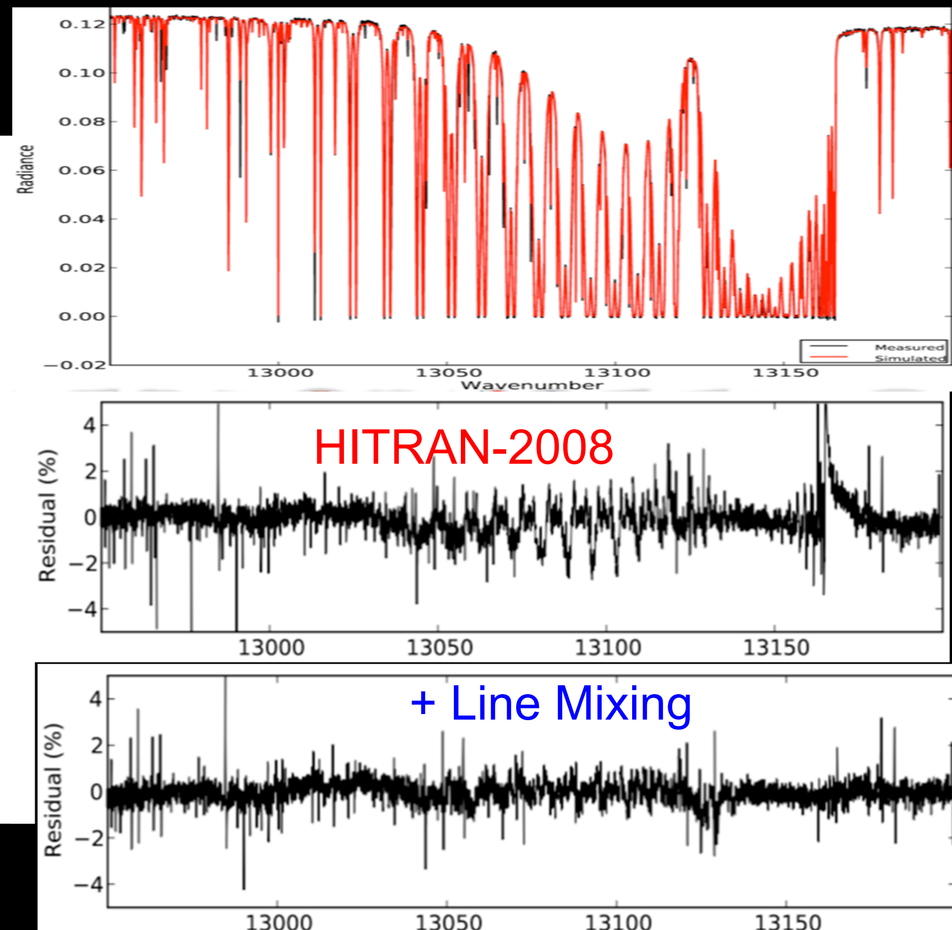
	0.76µm O_2	1.61µm CO_2	2.06µm CO2
Table range, resolution	12745-13245 cm^{-1}, 0.01cm^{-1} tables_v310.config	4700-6500cm^{-1}, 0.01cm^{-1} tables_v310.config	4700-6500cm^{-1}, 0.01cm^{-1} tables_v310.config
Positions	Robichaud (2008a, 2009)[1,2] line_mixing/o2/lm_o2_inputs_20091029/SDF.dat HITRAN08-o2mod.bin	Devi (2007)[1] HITRAN08.bin	Toth (2008)[1] HITRAN08.bin
Intensities	Robichaud (2008b, 2009)[1,2] line_mixing/o2/lm_o2_inputs_20091029/SDF.dat HITRAN08-o2mod.bin	Devi (2007)[1] HITRAN08.bin	Toth (2008)[1] HITRAN08.bin
Air-widths	Robichaud (2008)[1,2] line_mixing/o2/lm_o2_inputs_20091029/SDF.dat HITRAN08-o2mod.bin	Predoi-Cross (2009)[1] HITRAN08.bin	Predoi-Cross (2009)[1] HITRAN08.bin
Air-shifts	**Brown (2009) - R Branch only[3]** **line_mixing/o2/20091029/SDF.dat** Robichaud (2008a)[1,2] Predoi-Cross (2008)[1,2] HITRAN08-o2mod.bin	Devi (2007b)[1] HITRAN08.bin	Toth (2007)[1,4] HITRAN08.bin
Temperature dependence	Brown (2000)[1,2] line_mixing/o2/lm_o2_inputs_20091029/SDF.dat HITRAN08-o2mod.bin	Predoi-Cross (2009)[1] HITRAN08.bin	Predoi-Cross (2009)[1] HITRAN08.bin
Line shapes	Voigt[4]	Voigt[4]	Voigt[4]
Isotopic abundances	Rothman (2009), Šimečková (2006)[1,4,6] line_mixing/o2/lm_o2_inputs_20091029/SDF.dat HITRAN08-o2mod.bin	Rothman (2009), Šimečková (2006)[1,6] HITRAN08.bin	Rothman (2009), Šimečková (2006)[1,6] HITRAN08.bin
H_2O-broadened CO_2 widths	n/a[4] Fanjoux et al. (1994)	n/a[4] Sung (2009)	n/a[4] Sung (2009)
Air-Line mixing	Tran (2008) line_mixing/o2/lm_o2_inputs_20091029/RMF.dat	**Hartmann (2009)[5]** **line_mixing/co2/***	**Hartmann (2009)[5]** **line_mixing/co2/***
" " Temp. dependence	Tran (2008)	n/a	n/a
Narrowing	n/a[4]	n/a	n/a
CIA	Tran (2008) line_mixing/o2/lm_o2_inputs_20091029/CIAF.dat	n/a	n/a

O_2 A-band Spectroscopy

- Neglecting Line Mixing causes ~3% biases in retrieved O_2.

- Galatry vs. Voigt Line Shape: Voigt can introduce biases.





Solar Model

- The OCO forward model calculates the solar spectrum based on 2 subroutines:
  1) A solar continuum model based on a fit to SOLSPEC (Thiullier et al, 2003)
  2) A solar transmittance model, which reads an empirical solar linelist, which currently contains ~ 20,000 lines covering 550-15000 cm^{-1}.

- Solar Linelist is based on:
  - ATMOS exo-atmospheric spectra 550-4850 cm-1 (Geller, 1992)
  - MkIV balloon spectra, 650-5650 cm^{-1}
  - Kitt Peak ground-based solar spectra 5000-15000 cm^{-1}.

- Why use a solar model, rather than a measured solar spectrum?
  1) Solar spectrum is calculated on the exact spectral grid needed, avoiding the complication of re-sampling the measured spectrum.
  2) More flexibility in accommodating changes in the solar spectrum, with respect to time, or with respect to position on the solar disk.
  3) Can handle disk-center (e.g. FTS) or disk-integrated cases.

- Validation using GOSAT data ongoing.

Rayleigh Scattering

- Extinction per molecule based on classic equation (eg Van de Hulst 1957)

$$\sigma = \frac{24\pi^3(n_s^2 - 1)^2}{\lambda^4 N_s^2(n_s^2 + 2)^2}\left(\frac{6 + 3\rho}{6 - 7\rho}\right),$$

- Index of refraction using parameterization of Peck and Reeder (1972), with updates for increased CO2 based on Bodhaine et al (1999).
- Depolarization Factor assumed constant at 0.0279 (Young, 1981).
- Scattering Phase Matrix including polarization and dependence on the depolarization factor is based on a standard representation.

Clouds and Aerosols

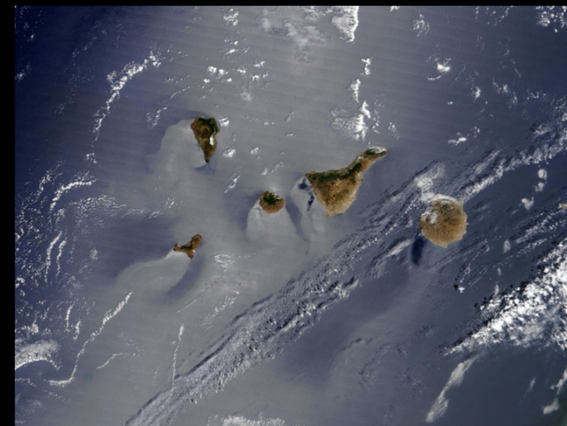
• Water clouds are parameterized as Mie spheres with desired effective radius and simple gamma distribution of particle sizes.

• Ice Clouds properties taken from Baum et al. (2005a,b), with phase functions truncated at 10° to reduce the very strong forward peak. Also parameterized according to effective radius, from 5-100 microns.

• Various aerosol types can also be included. We have calculated optical properties for 13 representative aerosol mixtures (Kahn et al, 2001).

• All scattering properties (ssa, phase matrix) assumed to vary linearly across a narrow OCO band.

Surface Properties



- ***Land:*** Simple lambertian albedo, taken to be a polynomial function of wavelength across an OCO band. (standard assumption is linear)

- ***Ocean:*** Fully-Polarized Cox-Munk model, dependent upon index of refraction of ocean surface and wind speed. This can be easily modified if data warrant.

Radiative Transfer Model

Stokes quantities (I, Q, U) are calculated on a high-resolution grid, as follows:

First-order of scattering RT: TMS correction (Nakajima & Tanaka, 1988) for I

$$I \approx I_{ss,tms} + I_{ms,dm}$$

$$Q \approx Q_{ss,exact} + Q_2$$

$$U \approx U_{ss,exact} \quad U_2$$

FAST ***SLOW***

LIDORT: Discrete-ordinate scalar RT

Natraj and Spurr, 2007: Fast, 2-orders of scattering polarized RT

- All 3 bands require ~ 25,000 spectral points.
- Speed improved using Low-Stream Interpolation (O'Dell, 2010)

Low-Accuracy Calculations (fast)
- Exact calculation for I_1,Q_1,U_1
- 2-stream multiple-scattering for I at degraded vertical resolution

~25,000 hi-res spectral points

High-Accuracy Calculations (slow)
- Exact 1st of scattering for I_1,Q_1,U_1
- 16-stream calculation for I,Q_2,U_2

~ 60 binned points

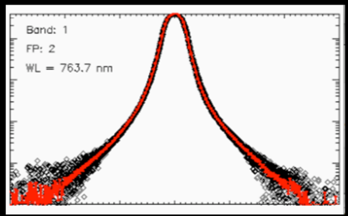
Instrument Model

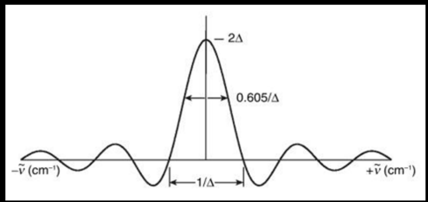
- High resolution Stokes parameters are combined via the instrument Stokes Coefficients to account for polarization sensitivity of the instrument:

$$I_{meas}(\lambda) = M_I\, I(\lambda) + M_Q\, Q(\lambda) + M_U U(\lambda)$$

- High-resolution $I_{meas}(\lambda)$ is then convolved with the instrument lineshape function (ILS) for each channel.

OCO ILS





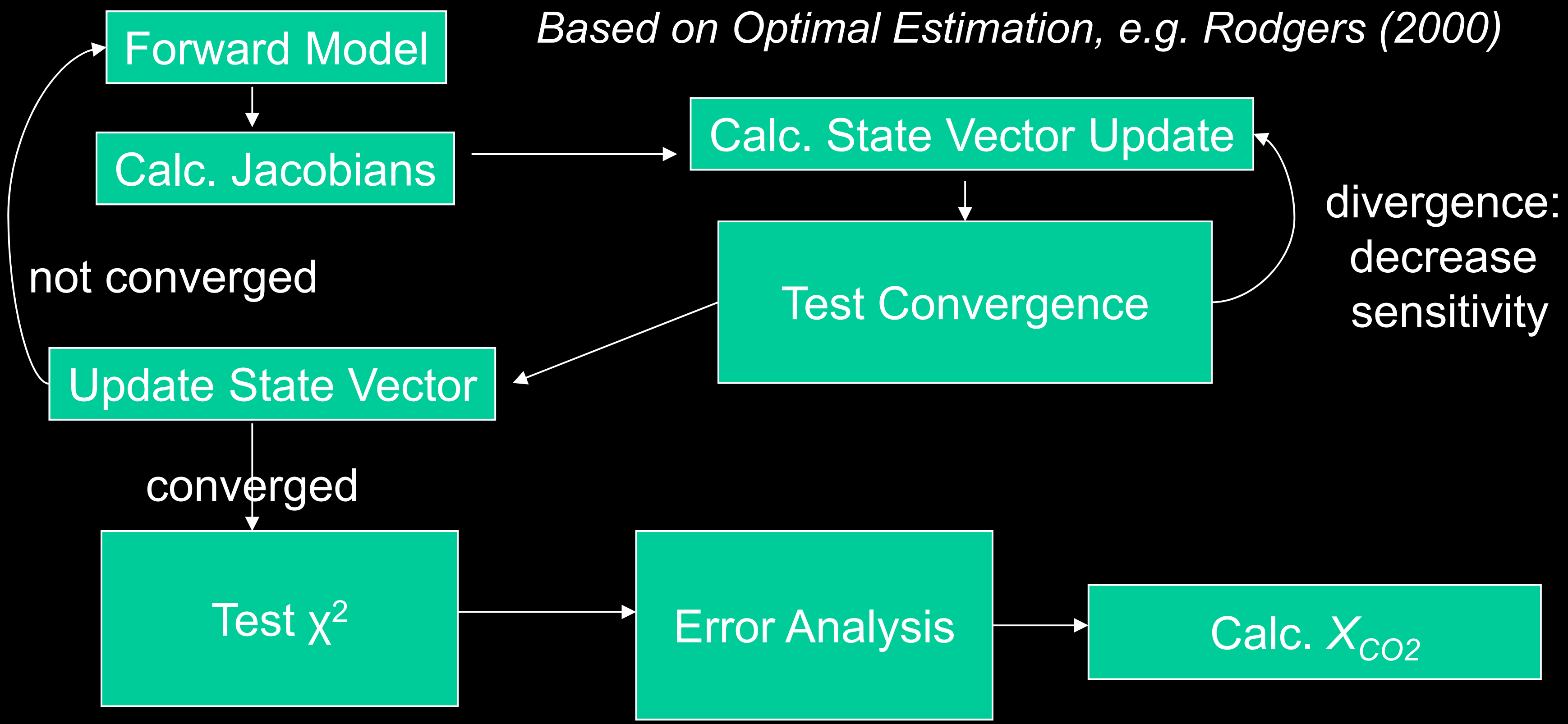
GOSAT ILS

- The location of the center of each ILS is described by the instrument's ***spectral dispersion***, modeled as a simple polynomial in channel index:

$$\lambda_i = d_0 + d_1\, i + d_2\, i^2 + \ldots$$

Inverse Method

Based on Optimal Estimation, e.g. Rodgers (2000)

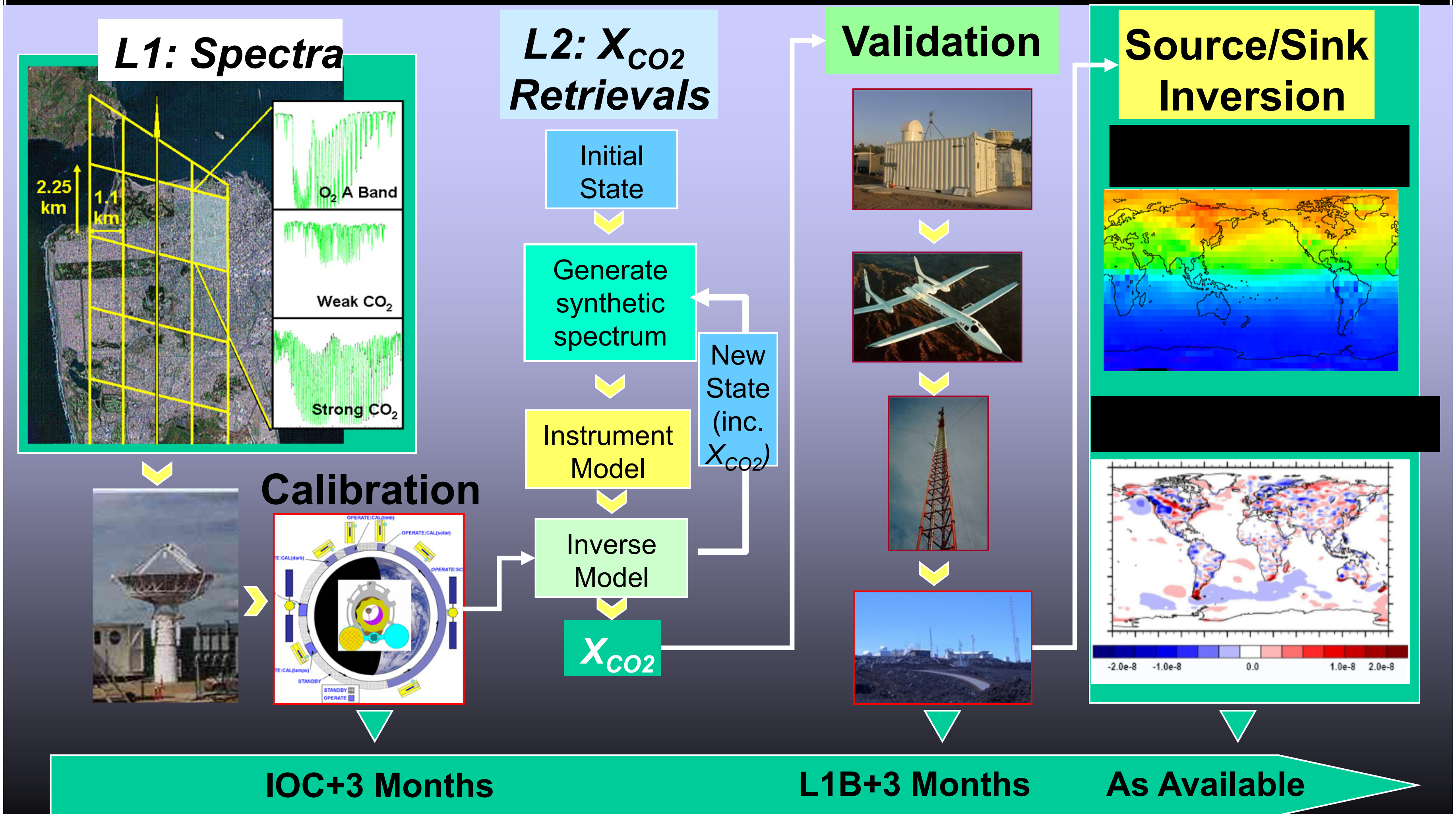


$$dx_{i+1} = \left((1+\gamma)S_a^{-1} + K_i^T S_\varepsilon^{-1} K_i \right)^{-1} \left[K_i^T S_\varepsilon^{-1} (y - f(x_i)) + S_a^{-1}(x_i - x_a) \right]$$

Products Recorded with each Sounding

Name	Size	Comment
χ^2	3	Sum of squares of normalized residuals in each spectrometer
	n	Retrieved State Vector
$\hat{\mathbf{S}}_{\mathbf{ii}}$	n	Diagonal elements of $\hat{S}$ (error covariance matrix)
$\hat{S}_{CO2}$	q^2	CO_2-only sub-matrix of $\hat{S}$
$_1$	n-q	Correlation of X_{CO2} with non-CO_2 elements of **x**
$\mathbf{A}_{\mathbf{CO2}}$	q^2	CO_2-only sub-matrix of averaging kernel (**A**)
$\mathbf{a}_{\mathbf{CO2}}$	n	Column averaging kernel
$\tilde{\mathbf{a}}_{\mathbf{c}}$	n	Error in X_{CO2} due to smoothing and interference
X_{CO2}	1	Column-weighted CO_2 dry air mole fraction
$\sigma^2{}_m$	1	Variance of X_{CO2} due to measurement noise
$\sigma^2{}_s$	1	Variance of X_{CO2} due to smoothing
$\sigma^2{}_i$	1	Variance of X_{CO2} due to interference
$\sigma^2{}_{XCO2}$	1	Total Variance of X_{CO2} ($\sigma^2{}_m + \sigma^2{}_s + \sigma^2{}_i$)
d_f	1	Degrees of Freedom (full state vector)
d_{CO2}	1	Degrees of Freedom (CO_2 profile only)

Data Product Delivery



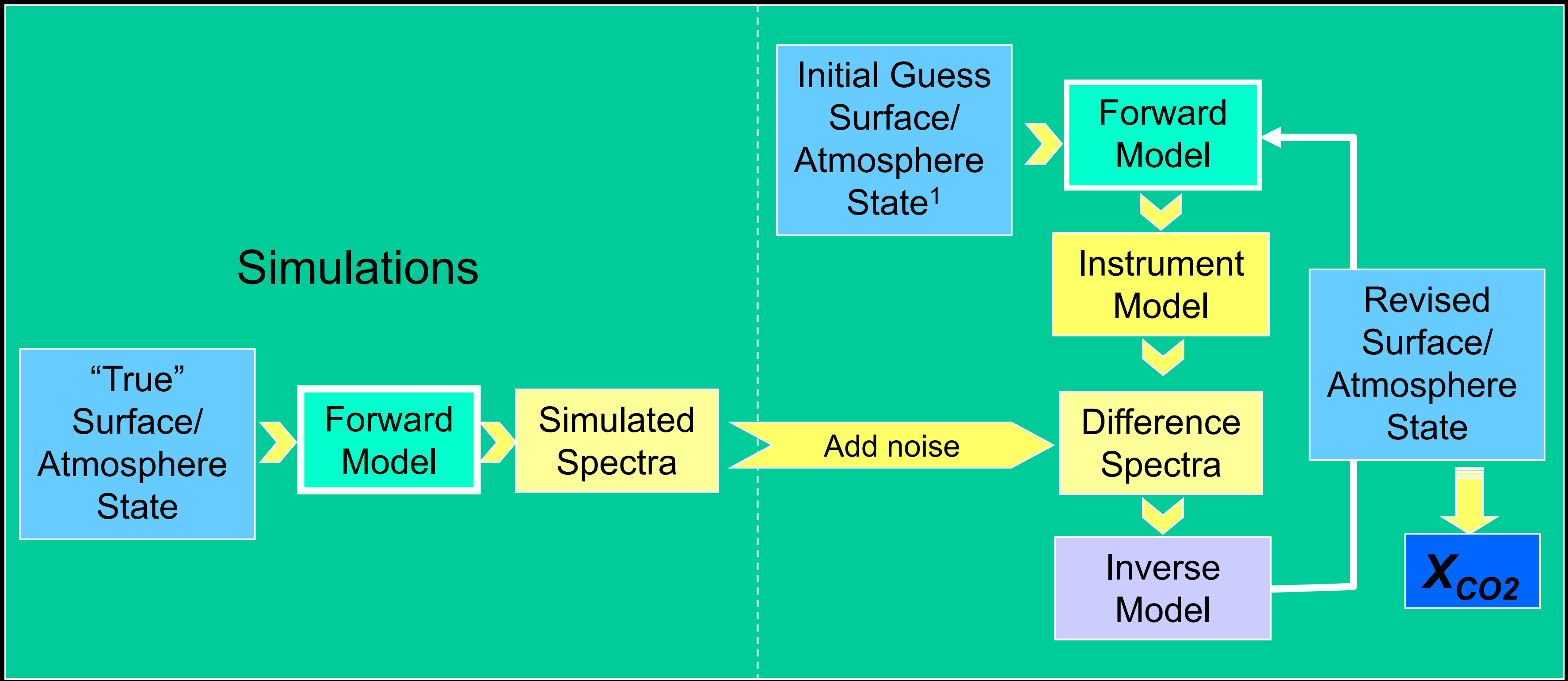
Testing the Retrieval Algorithm

- Two complementary methods are used to test the retrieval algorithm

  – Baseline tests:
    - how well the algorithm does when there are no “unknown” errors
      - Assess information content of spectra, as a function of instrument performance
      - Assess impact of clouds, aerosols, low surface albedos, etc. on retrievals
    - Uses a “simulator” based on a different Forward Model than that used by in the retrieval algorithm

  – GOSAT data processing:
    - Impact of realistic errors and biases
    - Validation against TCCON data and other datasets

Baseline Testing Approach



- *Different Forward Models are used for simulations and Full Physics retrievals*
- *Realistic levels of noise and other artifacts (e.g. residual image) are added to the simulated spectra*
- *The Initial guess of state vector is a perturbed version of "true" state.*

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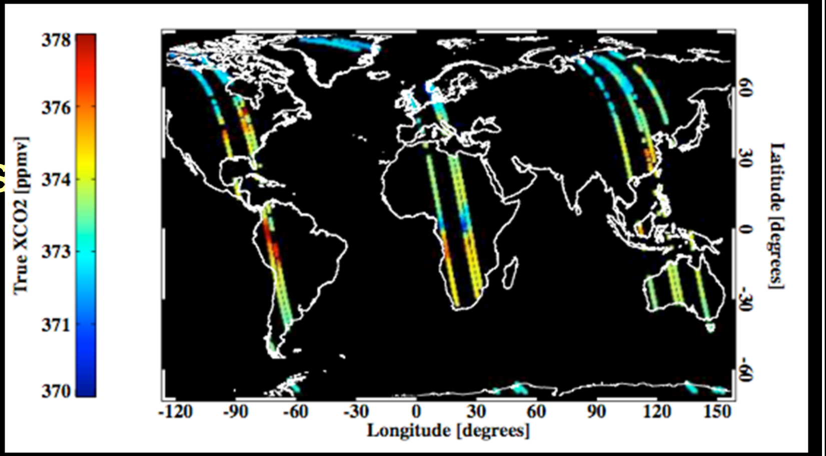
OCO Simulator

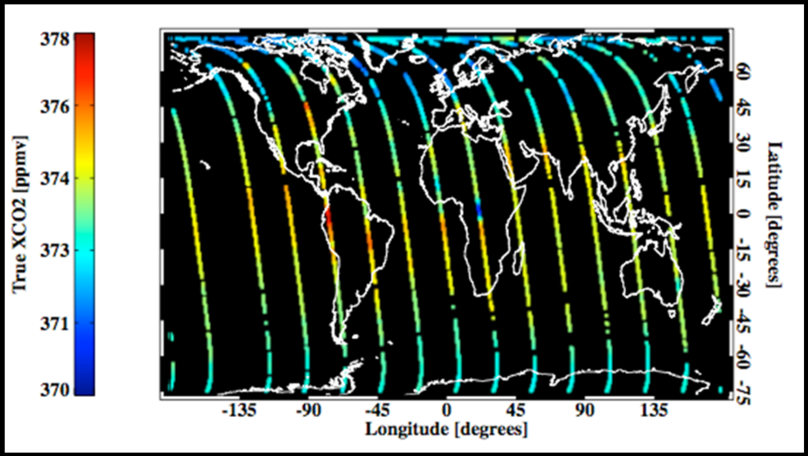
Includes:

- A-Train Orbital Paths
- Realistic, polarized land-surface BRDFs
- Cox-Munk ocean with foam component
- Cloud water & ice from CloudSat observations
- Aerosol distributions from Calipso (7 types)
- ~ 100 vertical layers
- T,q profiles from 60-layer ECMWF forecast
- Doppler shifts
- Slightly different RT model
- Ability to simulate nadir, glint, & target modes.

Nadir Orbits

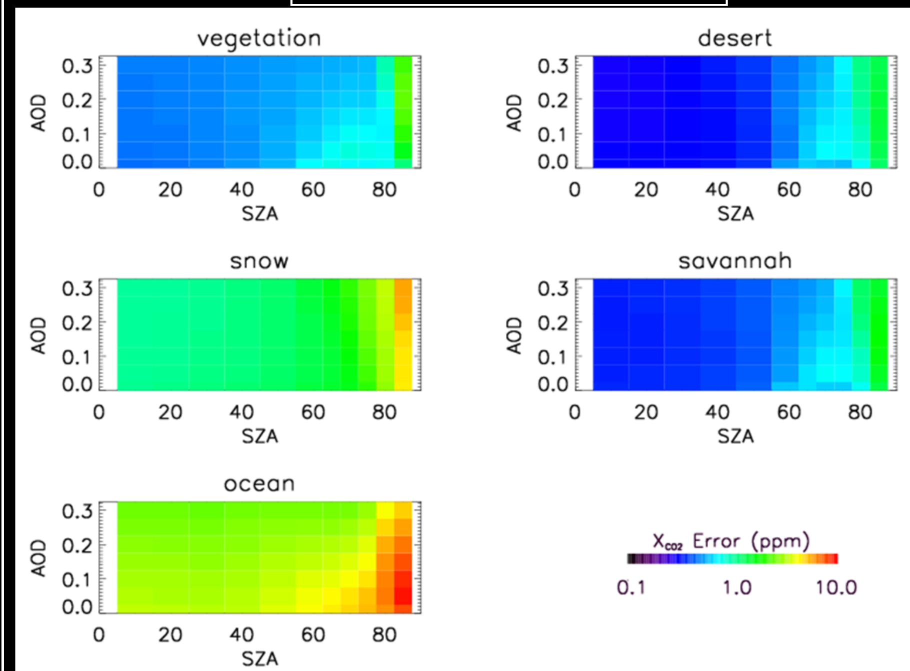


Glint Orbits

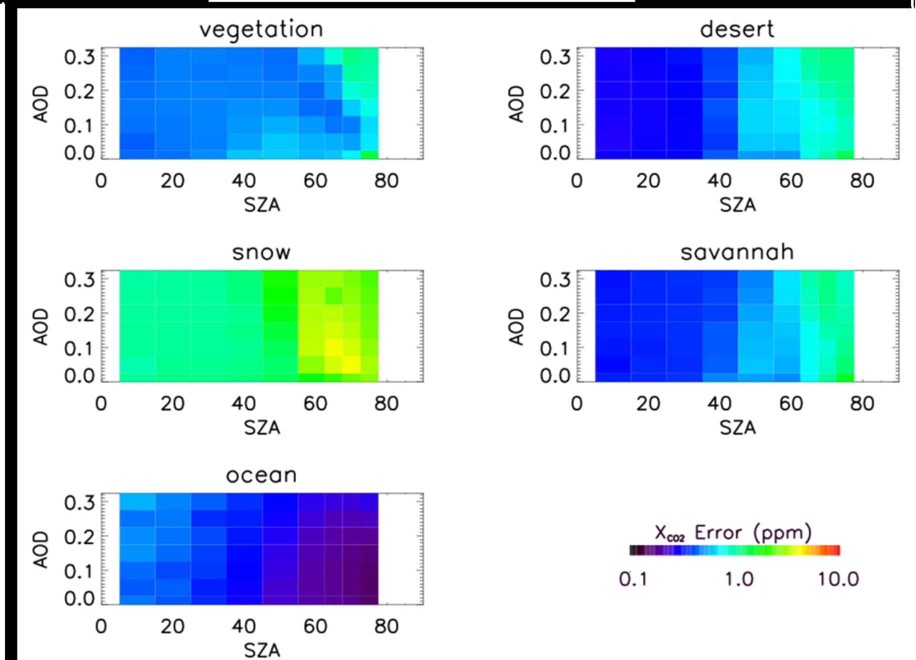


Linear Error Analysis Results: Single Sounding X_{CO2} Characterization

Nadir Retrieval Error



Glint Retrieval Error

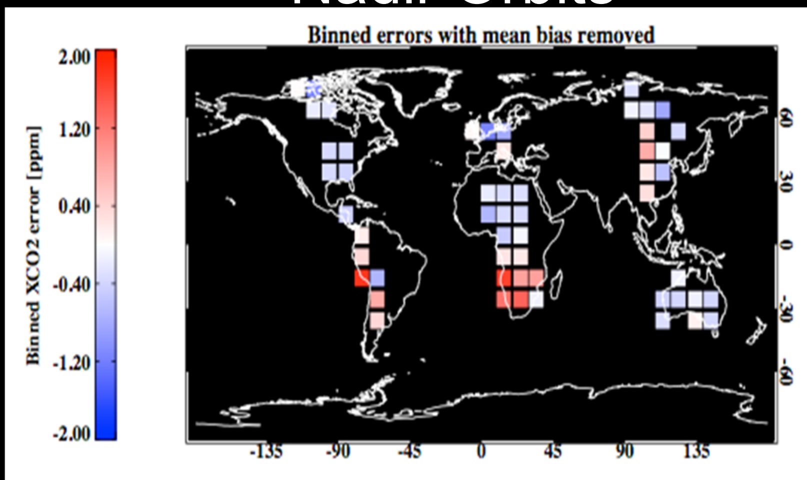


Linear Error analysis used to characterize the errors for nadir and glint observations

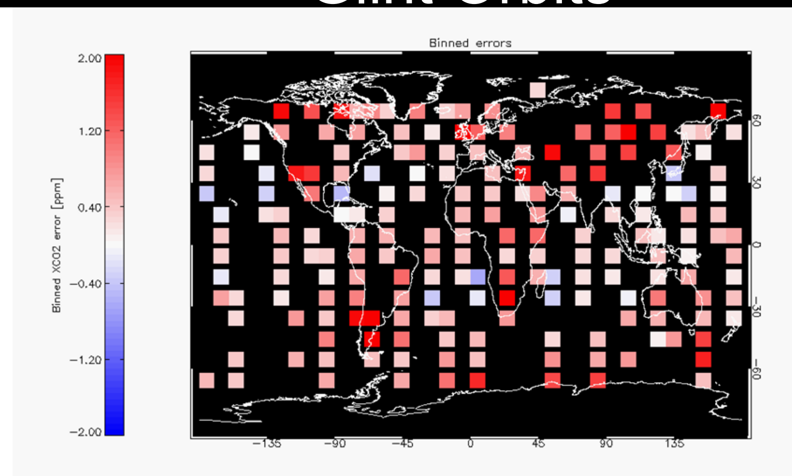
- Nadir observations are compromised by random errors associated with low instrument SNR when surface reflectance is low, and **solar zenith angles (SZA)** are large. These errors are enhanced by optical path length uncertainties when **aerosol optical depth (AOD)** are large
- Sun glint observations provide much higher SNR over ocean, which is dark at nadir

OCO Simulation Results

Nadir Orbits



Glint Orbits



All Land	**0.3 ± 2.8 ppm**
Good Land	0.4 ± 1.4 ppm

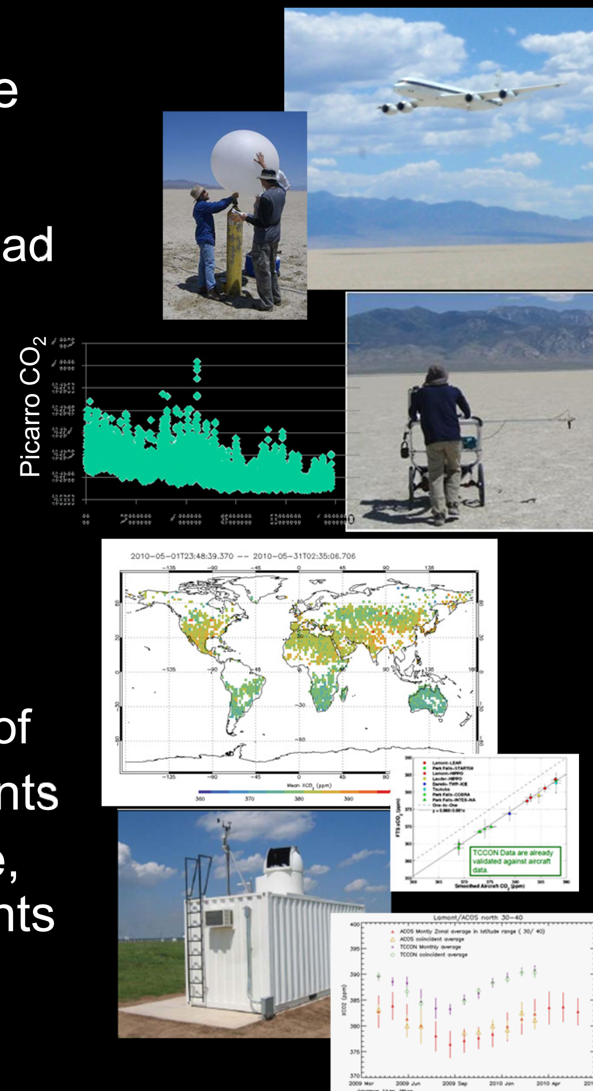
All Land	**0.4 ± 4.2 ppm**
Good Land	1.2 ± 1.4 ppm
All Ocean	0.2 ± 1.5 ppm
Good Ocean	0.3 ± 1.0 ppm

Experience Retrieving XCO2 from GOSAT Data

- Immediately after the loss of the OCO Mission, the GOSAT Project manager invited the OCO Team to participate in the GOSAT data analysis
- NASA reformulated the OCO team as the "Atmospheric Carbon Observations from Space" (ACOS) team
- This collaboration benefits the GOSAT team by:
  - Combining the ground based calibration and validation resources of both teams to maximize the accuracy of the GOSAT data
  - Combining the scientific expertise from both teams to accelerate our understanding of this new, space-based data source
- This collaboration benefits the NASA OCO by
  - Providing direct experience with the analysis of space based CO_2 measurements
  - Accelerating the delivery of precise CO_2 measurements from future NASA carbon dioxide monitoring missions

Elements of the ACOS/GOSAT Collaboration

- The ACOS team is collaborating closely with the GOSAT teams at JAXA and NIES to:
  - Conduct vicarious calibration campaigns in Railroad Valley, Nevada and analyze results of those campaigns
  - Retrieve X_{CO2} from GOSAT spectra
    - Model development, implementation, and testing
    - Data production and delivery
  - Validate GOSAT retrievals through comparisons of
    - GOSAT retrievals with TCCON measurements
    - 0ther validation standards (surface pressure, aircraft and ground-based CO_2 measurements

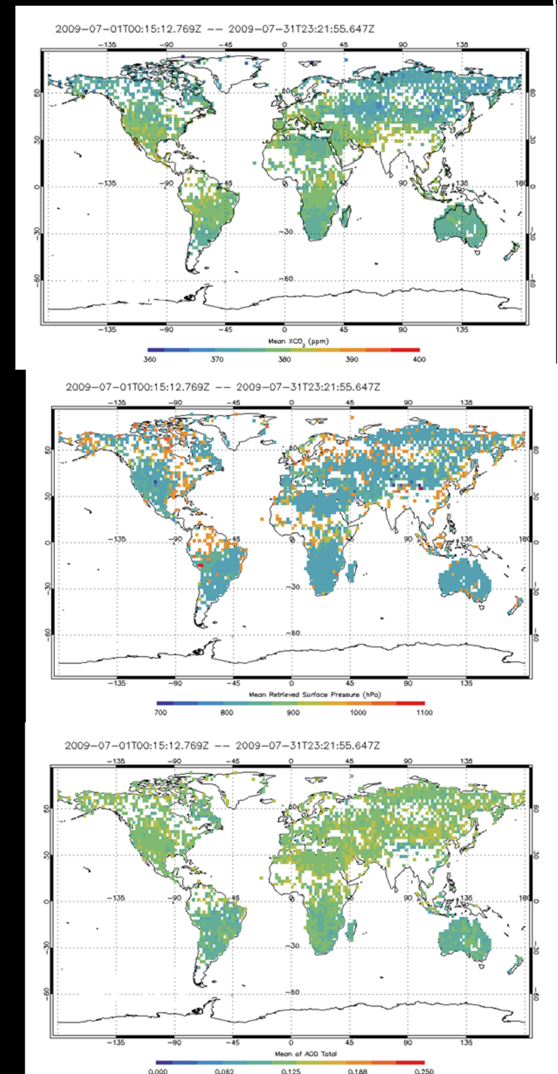


Preliminary Retrievals

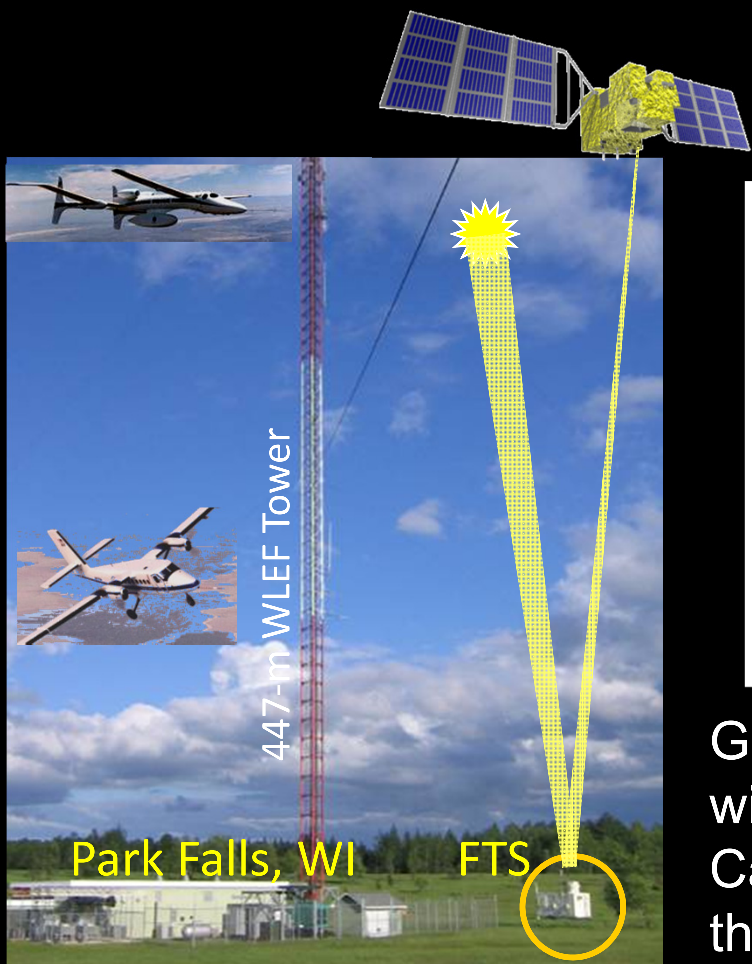
- An experimental ACOS “Standard Product” is currently being released from the GSFC DAAC

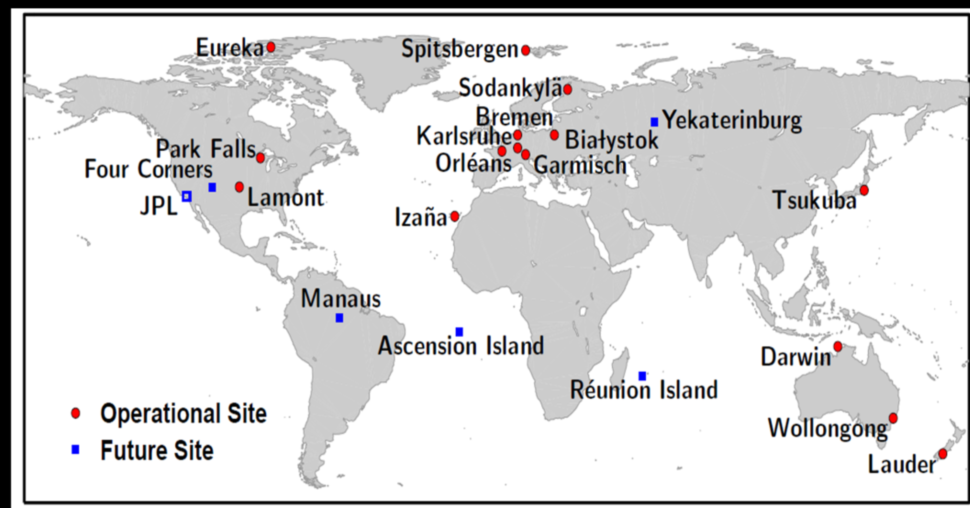
  http://mirador.gsfc.nasa.gov/

  - Until recently, only soundings over land were included in product
  - Ocean “glint” measurements have just started to become available in (January 2011)
  - Products include
    - The column-averaged dry air mole fraction, X_{CO2}
    - Other retrieved components of the surface/ atmosphere state vector (P_s, aerosol optical depth (AOD), surface albedo, etc.)
    - Averaging kernels and error estimates for each sounding



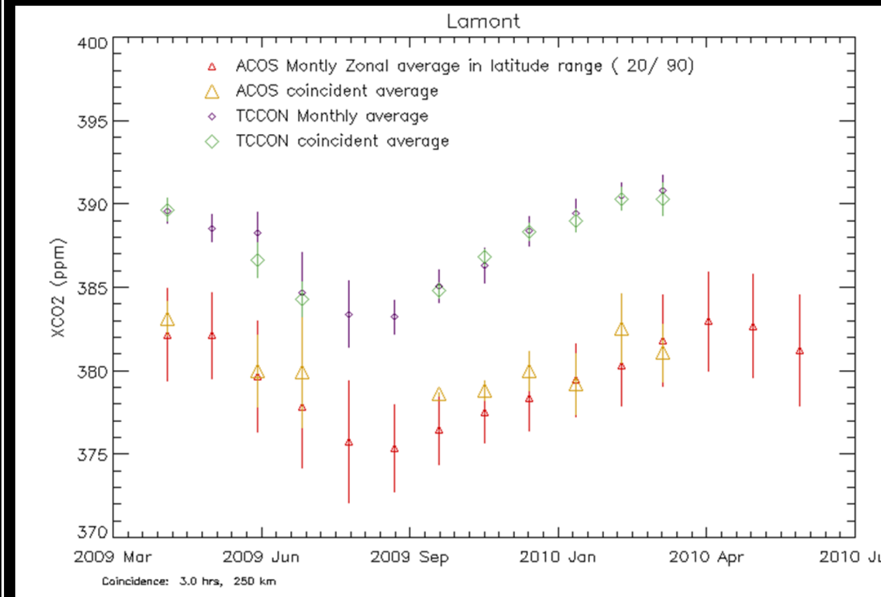
Validation of GOSAT Products





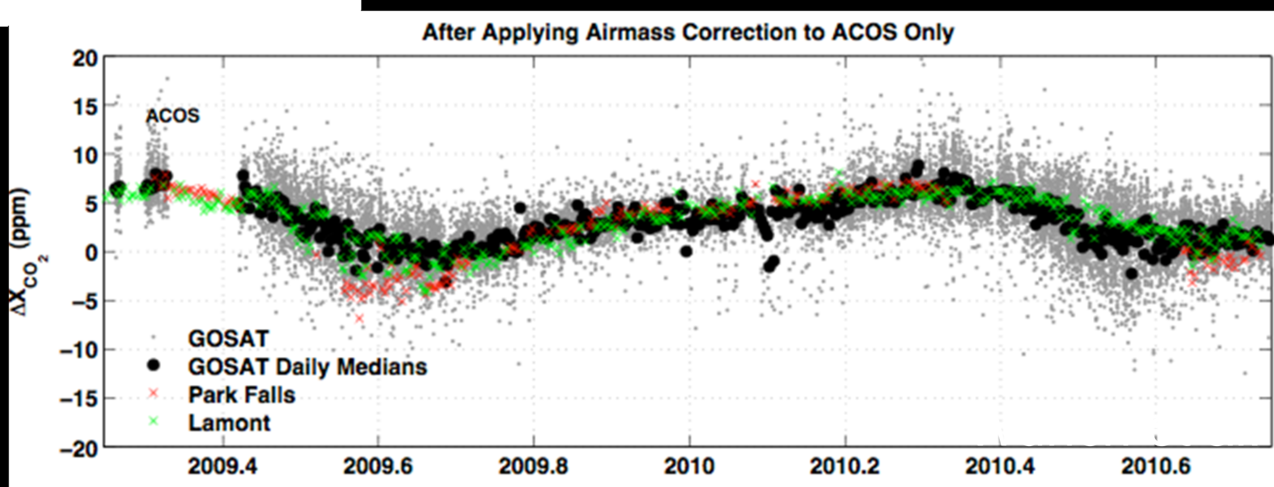
GOSAT X_{CO2} retrievals are being compared with those from the ground based Total Carbon Column Observing Network to very their accuracy

Comparisons of GOSAT and TCCON



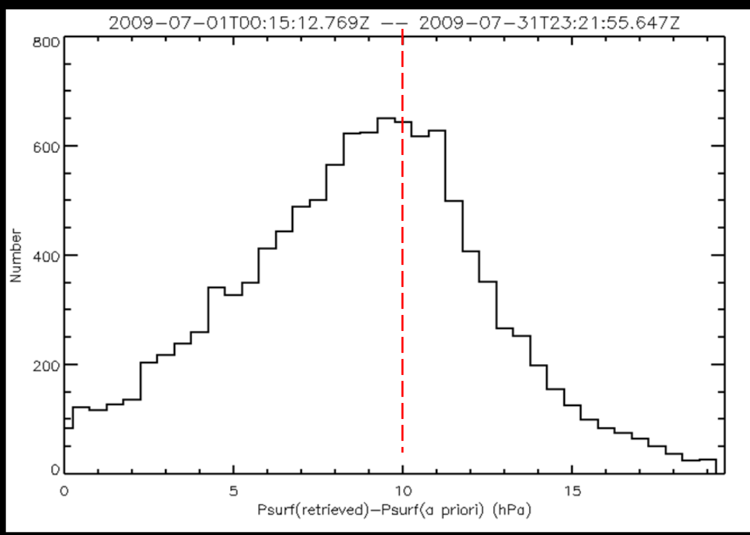
- ACOS GOSAT retrievals show
  - A consistent global bias of ~2% (7 ppm) in X_{CO2} when compared with TCCON and aircraft measurements.
  - A systematic air mass bias
  - X_{CO2} variations that are a factor of 2 to 3 larger than that measured by TCCON.

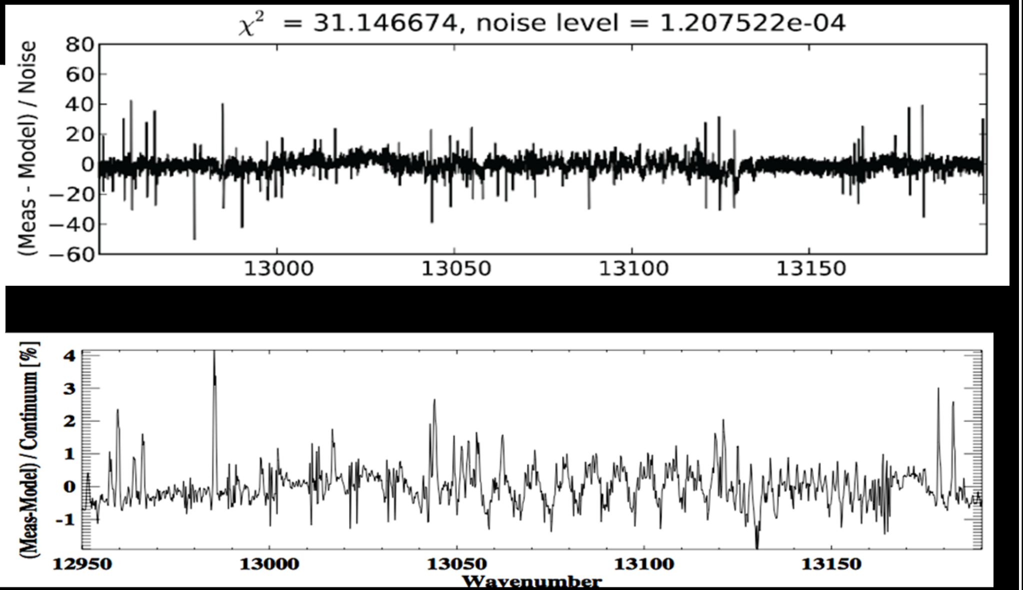
When the global and airmass biases are removed, the ACOS/GOSAT X_{CO2} retrievals do a good job of simulating the seasonal cycle over North America



Biases in the X_{CO2} Maps

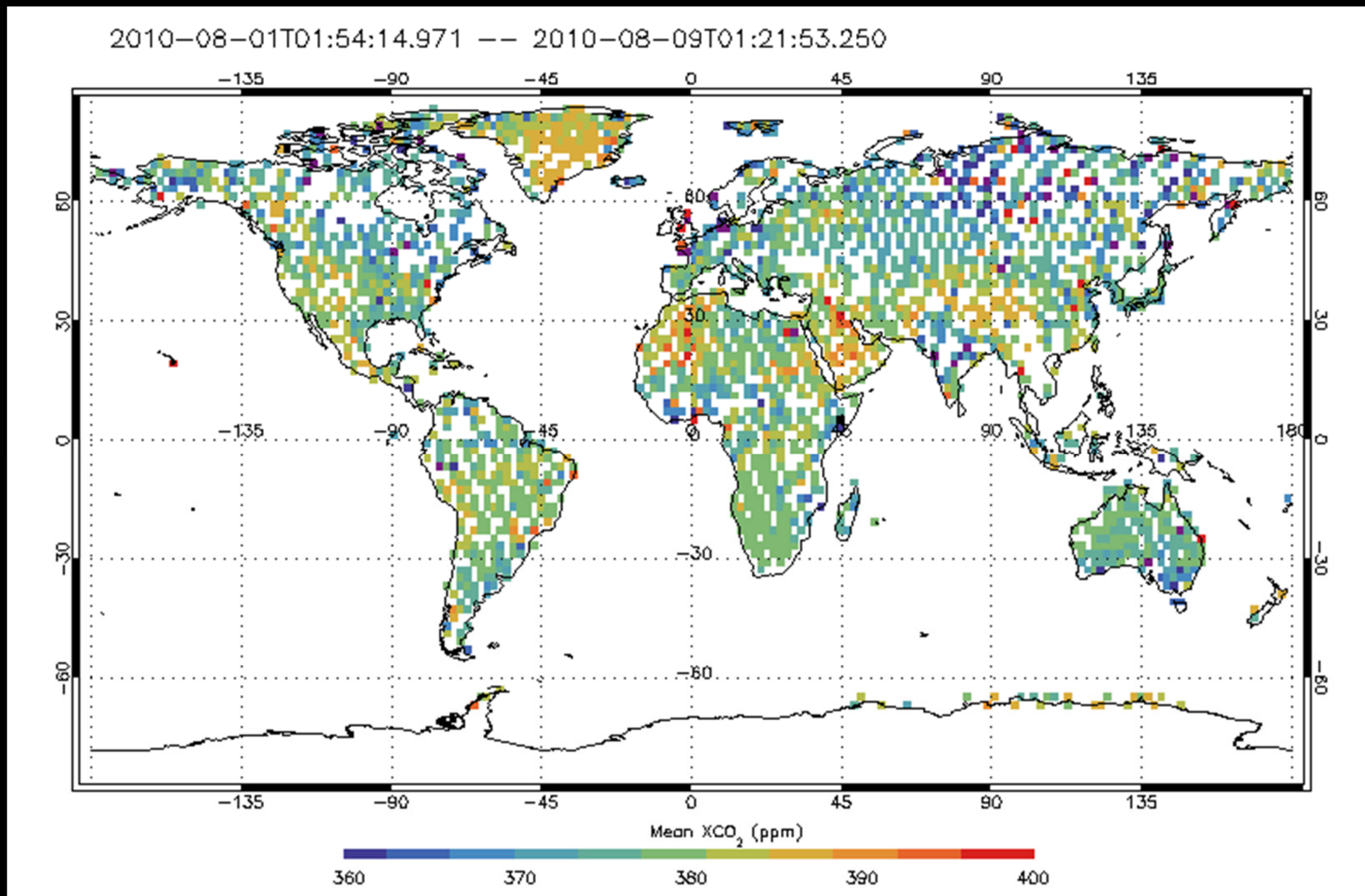
- A ~10 hPa (1%) high surface pressure bias contributes ~2/3 or the bias
- This bias may be associated with
  - Radiometric and spectroscopic calibration errors in the L1B data
    - Several corrections currently being tested
  - Line mixing, line shape or other issues with the O_2 A-band absorption cross sections





Typical O_2 A-band retrieval residuals.

Unscreened GOSAT Retrievals for 1-8 August 2010 (includes some cloudy data)



Unscreened X_{CO2} retrievals from 1-8 August also show anomalously high values over the Sahara Desert (due to dust contamination), but enhanced CO_2 near Moscow.

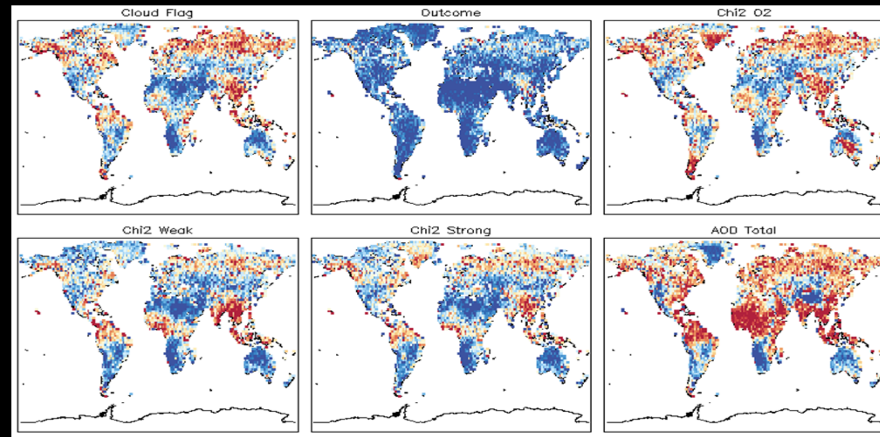
Post Screening Improves Accuracy

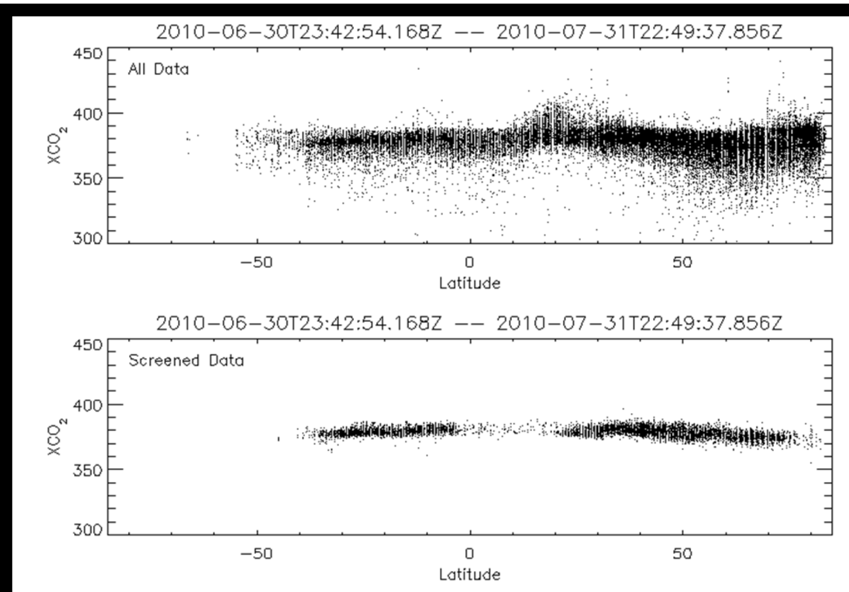
Errors can be further reduced by post-screening retrievals, based on a series of criteria, including:

- Measurement SNR
- Convergence
- Goodness of spectral fit
- Surface pressure error
- Evidence for clouds or optically thick aerosols
- A postiori retrieval error
- Evidence of known biases

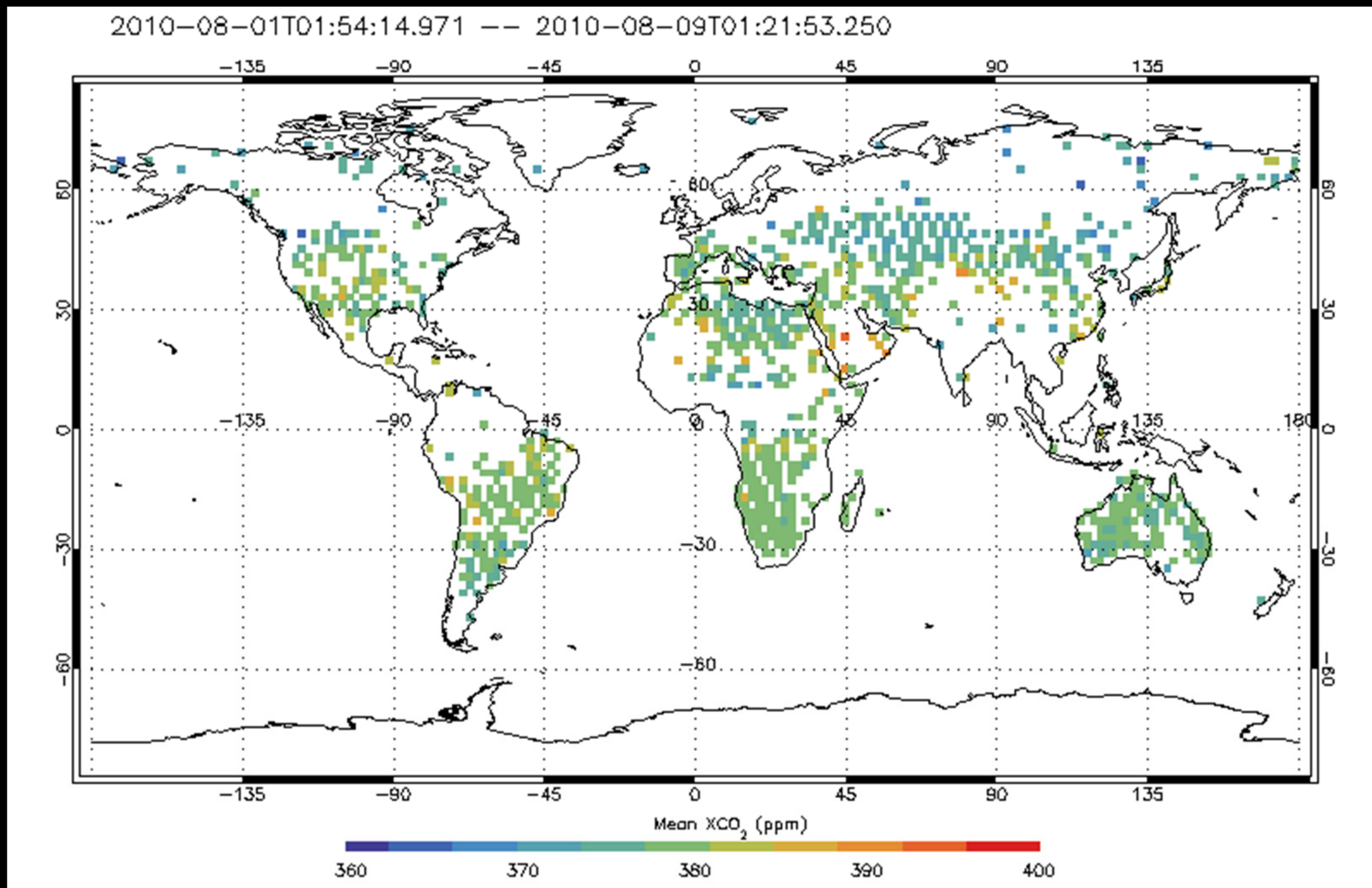
The cloud screen is responsible for the largest data reductions.

- Improved cloud screening algorithms are a major focus of our development effort





Screened GOSAT L2 Products for 1-8 August 2010 (Vigorous Cloud and Data Quality Screening)



Screening removes anomalous dust contaminated values over the Sahara, but also removes most data north of 50 degrees latitude.

Conclusions

- The OCO-2/ACOS retrieval algorithm
  - is currently in place and is generating a production product for GOSAT
  - Is still evolving, to address know errors and biases

- The ACOS/GOSAT collaboration is beginning to return benefits to both teams
  - The vicarious calibration experiments have helped to identify and correct for changes in the pre-launch GOSAT radiometric calibration parameters.
  - Comparisons with TCCON measurements have revealed a global, -2% bias in the preliminary ACOS X_{CO2} retrievals
  - Comparisons between surface pressure retrievals and the ECMWF prior indicate that about half of this bias can be attributed to a +10 hPa bias in the retrieved surface pressure

- Lessons learned from this experience are expected to substantially accelerate the delivery of high quality products from the OCO-2 mission, which is currently scheduled for launch in February 2013